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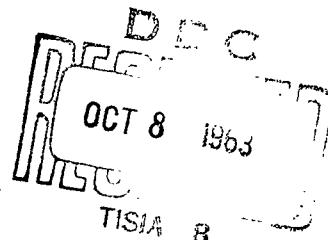
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Abstract for International Crystallographic Convention, Leningrad, U. S. S. R.,
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Crystal-Structural Mechanism
of the Ferroelectric Behavior
of (Glycine)₃·H₂SO₄*

Ray Pepinsky,
Department of Physics
The Pennsylvania State University
University Park, Pa.,
and
Brookhaven National Laboratory
Upton, Long Island, New York, U. S. A.



Ferroelectric (glycine)₃·H₂SO₄¹ crystallizes at room temperature in the monoclinic system with $a = 9.417$ Å, $b = 12.643$ Å, $c = 5.735$ Å, $\beta = 110^\circ 23'$; the space group is $P2_1$, and the polar direction is along the two-fold screw axis. Above 47°C the spontaneous polarization disappears as the space group becomes $P2_1/m$. The crystal structure was determined from full three-dimensional x-ray diffraction data, using $\text{CuK}\alpha$ radiation.² Out of the three glycine molecules in the crystal, one has the usual zwitterion configuration, with the NH_3^+ group out of the plane of the other atoms; the remaining two glycines are mono-protonated, and planar within experimental error, and are designated as glycinium ions. Thus the chemical formula is properly written as $(\text{NH}_3^+\text{CH}_2\text{COO}^-) \cdot (\text{NH}_3^+\text{CH}_2\text{COOH})_2 \cdot \text{SO}_4^{--}$, and the compound is best described by the chemical name glycine diglycinium sulfate. One of the planar glycinium ions lies near but not in the plane $y = 1/4$, which becomes the mirror plane in the high-temperature phase. There is disorder in this arrangement, even below the Curie point and down to a temperature of -70°C .

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The nitrogen atoms form N-H··O hydrogen bonds of the usual strength, whereas a quite strong O-H··O hydrogen bond with a distance of 2.43₈ Å is found between the oxygen atom of the carboxyl group of the zwitter-ion glycine and that of the planar glycinium ion which lies near the plane $y = 1/2$. This hydrogen is not in a central potential well; and its shift from one carboxyl group to the other, as the polarization direction is reversed, is accompanied by changes in the stereochemistry of the ions, and by other marked changes in the entire structure. These are described.

Above the Curie point, at 47°C, mirror symmetry is attained by full statistical arrangement of molecules around the mirror planes at $y = 1/4$ and $3/4$.

The structure has been studied by the Okaya-Pepinsky $P_s(u)$ function,³ using proportional-counter measurements of scattered CuK α radiation;⁴ and the effect of the imaginary part of the sulfur structure factor is sufficient to yield the entire structure. The absolute configuration and direction of structural polarization under an applied electric field is established, therewith.

A neutron analysis⁵ has confirmed the x-ray results, and has established the positions of all hydrogen atoms. In particular, the neutron study reveals the non-centered position of the hydrogen between glycine ions near the $y = 1/2$ plane, and confirms the differences in stereochemistry between the zwitter-ion and monoprotonated glycines.

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